Nonylphenyl diphenyl phosphate, mixed isomers

64532-97-4 | DTXSID4025797

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.17e-06 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.16e-01

Confidence level: 5.50e-01

Nearest Neighbors from the Training Set

Image not found
Octyl diphenyl phosphate
Measured: 3.86e-07
Predicted: 4.44e-05

Image not found
2-Ethylhexyl diphenyl phosphate
Measured: 5.24e-06
Predicted: 4.50e-05

Image not found
Tris(2,3-dibromopropyl) phosphate
Measured: 1.15e-05
Predicted: 1.88e-05

Image not found
Acrinathrin
Measured: 3.69e-08
Predicted: 8.12e-05

Image not found
Aspon
Measured: 7.93e-05
Predicted: 6.58e-05